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SCATTERED WAVE FUNCTIONS OF DISLOCATED LATTICES

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Using a Wannier function approach and a transformation of the coordinate system it is shown that a method can be set up to calculate the scattered wave function of a dislocated lattice.

The electronic states within condensed matter are of fundamental importance. In fact, no quantitative estimate of any property of a semiconductor, metal or insulator on the basis of first principles can be made without information about these states.

In the past, most of the investigations concerning the electronic state of dislocations were carried out for semiconductors [1, 2, 3]. The quantum mechanical consideration of such a complex system as a dislocation has been given on the basis of more or less drastically simplified models.

The presence of dislocations may notably increase the electrical resistivity of a metal. The change in electrical resistivity resulting from plastic deformation of metals has been measured by many workers [4, 5, 6], and several reviews on this subject have appeared. The most extended model known in the literature is the model of Huffman et al. [7] for metals which is based on the fact that dislocation motion in a metal induces an electric field by which currents in the conduction electron gas are caused.

To estimate the electronic states within the core of the dislocation, Harrison [8] assumed a hollow core consisting of a row of vacancies, which would seem physically implausible.

One of the problems for a quantum mechanical description of a dislocated lattice is to formulate compatible sets of incoming and scattered wave functions.

The following model gives a method for describing these wave functions.

The model is based on a transformation of the coordinate system \mathbf{r} describing the dislocation to a system $\mathbf{r}'(\mathbf{r})$ in which the positions of the atoms possess a periodicity with the exception of a gap. In fig. 1 the transformation has been depicted in the case of a cubic lattice. The model, however, is not restricted to simple cubic lattices nor to a particular dislocation-slip system. The circle C represents the cross section of a cylinder, with the dislocation line as axis. The radius of the circle C should be greater than the minimum interatomic distance. The z-axis of a coordinate frame is taken parallel to the dislocation line.

The solution of the one-electron problem for a perfect system without any dislocation is formulated in terms of Wannier functions [9]. The Hamiltonian is given by:

$$\mathcal{H}_0(\mathbf{r}) = T_0(\nabla) + V(\mathbf{r}), \quad \text{where } T_0(\nabla) = -(\hbar^2/2m)\nabla^2. \quad (1)$$

Bloch functions can be expressed in terms of Wannier functions [10]

$$\Psi_{n,\mathbf{q}}(\mathbf{r}, E_n) = \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \sum_{\mu} e^{i\mathbf{q} \cdot \mathbf{R}_{\mu}} a_n(\mathbf{r} - \mathbf{R}_{\mu}, E_n), \quad (2)$$

where $a_n(\mathbf{r} - \mathbf{R}_{\mu}, E_n)$ = Wannier function characterized by a band index n and the μ th lattice site vector \mathbf{R}_{μ} ; \mathbf{q} = wave vector, Ω = volume unit cell.

Wannier functions are not energy eigenfunctions. They are combinations of Bloch functions with differ-

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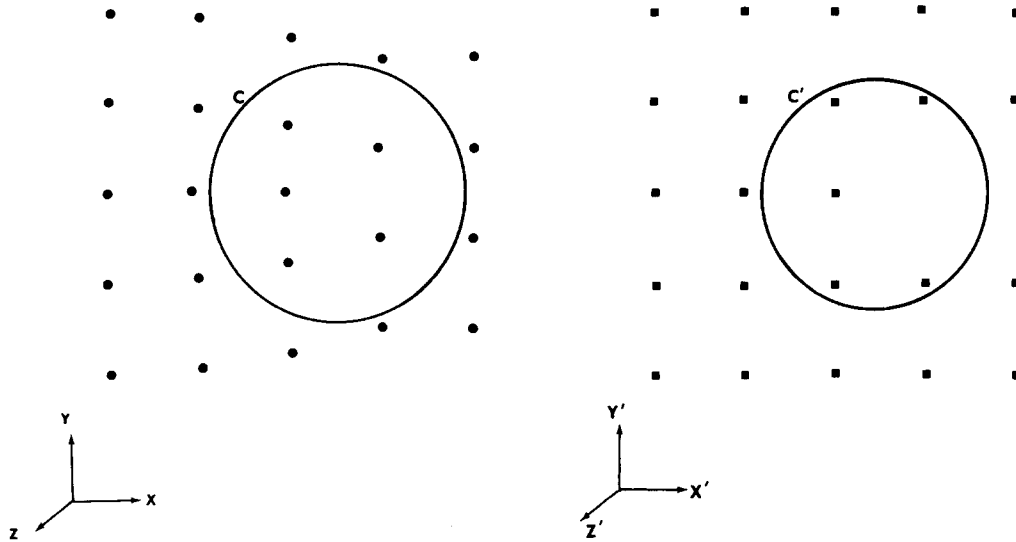


Fig. 1. Representation of the transformation C to C' system containing an edge dislocation in simple cubic lattices.

rent wave vectors and therefore different energies.

Using the properties of the Bloch functions, the following relation can be easily derived:

$$\mathcal{H}_0 a_n(\mathbf{r} - \mathbf{R}_\mu, E_n) = \sum_\nu \epsilon_n(\mathbf{R}_\nu - \mathbf{R}_\mu) a_n(\mathbf{r} - \mathbf{R}_\nu, E_n), \quad (3)$$

with

$$\epsilon_n(\mathbf{R}_\sigma) = \frac{\Omega}{(2\pi)^3} \int e^{i\mathbf{k} \cdot \mathbf{R}_\sigma} E_n(\mathbf{k}) d^3k. \quad (4)$$

The quantity $\epsilon_n(\mathbf{R}_\sigma)$ is a Fourier component of the energy-band function $E_n(\mathbf{k})$.

Outside the cylinder, a distorted solution will be used for the dislocated lattice. The Hamiltonian in the transformed \mathbf{r}' system can be written as:

$$\mathcal{H}(\mathbf{r}') = T_0(\nabla') + \Delta T(\nabla') + V(\mathbf{r}') = \mathcal{H}_0(\mathbf{r}') + \Delta T(\nabla'). \quad (5)$$

For the energy eigenfunctions in this region we take:

$$\begin{aligned} \Psi_n(\mathbf{r}', E'_n) \\ = \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \sum_\mu \exp[i\mathbf{q}(\mathbf{R}'_\mu) \cdot \mathbf{R}'_\mu] a_n(\mathbf{r}' - \mathbf{R}'_\mu, E_n), \end{aligned} \quad (6)$$

where E'_n represents the disturbed energy and $a_n(\mathbf{r}' - \mathbf{R}'_\mu, E_n)$ a Wannier function of the perfect system. Using eq. (5) and eq. (3), the following can

be written:

$$\begin{aligned} \mathcal{H}(\mathbf{r}') \Psi_n(\mathbf{r}', E'_n) \\ = \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \sum_\mu e^{i\mathbf{q}(\mathbf{R}'_\mu) \cdot \mathbf{R}'_\mu} \left\{ \sum_\nu [\epsilon_n(\mathbf{R}'_\nu - \mathbf{R}'_\mu) a_n(\mathbf{r}' - \mathbf{R}'_\nu)] \right. \\ \left. + \sum_{n'} \langle n' \nu | \Delta T | n \mu \rangle a_{n'}(\mathbf{r}' - \mathbf{R}'_\nu) \right\} = E'_n \Psi_n(\mathbf{r}', E'_n). \end{aligned} \quad (7)$$

The function $\mathbf{q}(\mathbf{R}')$ is chosen to satisfy

$$\mathbf{q}(\mathbf{R}'_\mu) \cdot \mathbf{R}'_\mu = \mathbf{q} \cdot \mathbf{R}_\mu. \quad (8)$$

Let D be the minimum of $|\mathbf{C}'|$. In the asymptotic solution one can state:

$$(\mathbf{R}'_\nu - \mathbf{R}'_\mu) \approx (\mathbf{R}_\nu - \mathbf{R}_\mu), \quad (9)$$

$$(\mathbf{r}' - \mathbf{R}'_\nu) \approx (\mathbf{r} - \mathbf{R}_\nu), \quad (10)$$

while

$$|\mathbf{R}'_\nu - \mathbf{R}'_\mu| \ll D, \quad (11)$$

$$|\mathbf{r}' - \mathbf{R}_\nu| \ll D. \quad (12)$$

Using eqs. (9) to (12), the perturbation in eq. (7) can be written as:

$$\begin{aligned} \langle n' \nu | \Delta T | n \mu \rangle &= \langle n' \nu(\mathbf{r}') | \Delta T(\mathbf{r}', \mathbf{r}) | n \mu(\mathbf{r}') \rangle \\ &= \langle n' \nu(\mathbf{r}') | T_0(\nabla') | n \mu(\mathbf{r}') \rangle - \langle n' \nu(\mathbf{r}') | T_0(\nabla) | n \mu(\mathbf{r}') \rangle, \end{aligned} \quad (13)$$

where $\langle n'v|$ and $|n\mu\rangle$ represent the localized states. In the asymptotic region

$$\langle n'v|\Delta T|n\mu\rangle \approx 0 \quad \text{and} \quad T_0(\nabla') = T_0(\nabla). \quad (14)$$

This implies:

$$\mathcal{H}(\mathbf{r}')\Psi_n(\mathbf{r}', E'_n) = E_n\Psi_n(\mathbf{r}', E'_n), \quad E'_n = E_n. \quad (15)$$

The wave function for the lattice containing a dislocation can now be given using eq. (8), eq. (10) and eq. (15) as:

$$\Psi_n(\mathbf{r}', E'_n) = \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \sum_{\mu} e^{i\mathbf{q}\cdot\mathbf{R}_{\mu}} a_n(\mathbf{r} - \mathbf{R}_{\mu}, E_n). \quad (16)$$

The scattered wave can be found analogously, using the part of \mathbf{q} perpendicular to the dislocation line:

$$\begin{aligned} \Psi_{n,sc}(\mathbf{r}', E'_n) = & \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \sum_{\mu} \left\{ e^{iq_z R_{\mu,z}} \right. \\ & \times \left. \frac{\exp(i|\mathbf{q}_{xy}||\mathbf{R}_{\mu,xy}|)}{|\mathbf{R}_{\mu,xy}|^{1/2}} f(\phi_{\mu}) \right\} a_n(\mathbf{r} - \mathbf{R}_{\mu}, E_n), \end{aligned} \quad (17)$$

where $f(\phi_{\mu})$ represents the scattering amplitude dependent on the polar angle of $\mathbf{R}_{\mu,xy}$. The vector \mathbf{R}_{μ} is equal to $\mathbf{R}_{\mu,xy} + R_{\mu,z}\mathbf{k}$, where \mathbf{k} represents the unit vector in the Z direction, i.e. along the dislocation line. Eq. (17) is analogous to the formulation in the case of a vacancy, as derived by Callaway [10, p. 392].

Inside the cylinder C the solution is:

$$\begin{aligned} \Psi_{ins}^n(\mathbf{r}, E_n) \\ = \sum_{\mu} e^{iq_z R_{\mu,z}} \sum_l \sum_{m=-l}^{m=+l} A_{lm}^{(\mu,xy)} h_l^{(1)}(\kappa|\mathbf{r}-\mathbf{R}_{\mu}|) Y_{lm}(\mathbf{r}-\mathbf{R}_{\mu}), \end{aligned} \quad (18)$$

where $h_l^{(1)}(\kappa|\mathbf{r}-\mathbf{R}_{\mu}|)$ represents the spherical Hankel function of the first kind, $Y_{lm}(\mathbf{r}-\mathbf{R}_{\mu})$ is the real

spherical harmonic, and $\kappa = (V(\mathbf{r}) - E_n)^{1/2}$. The wave functions for the region outside the cylinder can be written, using eq. (16) and eq. (17) as:

$$\begin{aligned} \Psi_{outs}^n(\mathbf{r}, E_n) = & \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \sum_{\mu} \left\{ e^{i\mathbf{q}\cdot\mathbf{R}_{\mu}} \right. \\ & + \left. \frac{\exp(iq_z R_{\mu,z}) \exp(i|\mathbf{q}_{xy}||\mathbf{R}_{\mu,xy}|)}{|\mathbf{R}_{\mu,xy}|^{1/2}} f(\phi_{\mu}) \right\} a_n(\mathbf{r}-\mathbf{R}_{\mu}, E_n). \end{aligned} \quad (19)$$

At the boundary C the values of the wave functions Ψ_{outs}^n , Ψ_{ins}^n as well as their derivatives have to be equal because of the requirement of continuity.

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